Thanks! This was helpful.

If you want lots of compounds with high drug scores, it would be better to let everything survive, then find the ones with the best drug score, then evolve those so that only those most similar to the parent compound (which have high drug scores to begin with) survive, with a small generation size, and lots of generations (we'd have to define where to stop unless you wanted to select unlimited). This way we would have high drug scores and diversity.

We decided to edit the source code so everything survives first.

I still have to graph generation number vs. drug score, but from what it sounds like when you use the genetic algorithm, the drug score may not be improving from the first generation to the last.

Thanks I will let you know if they have any more questions.